



The Relative Role of Local and Regional-Scale Processes on Ozone in Philadelphia

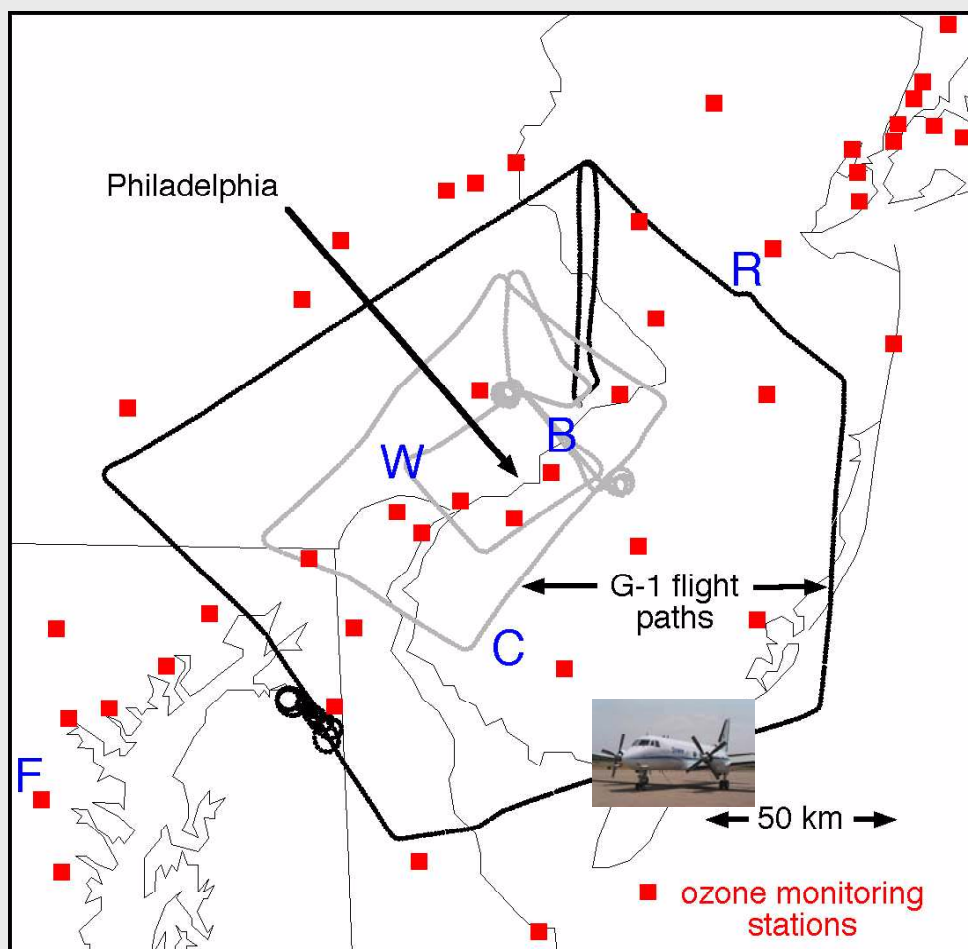
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with contributions from:

modeling: Xindi Bian, Carl Berkowitz, Elaine Chapman, Richard Easter, Rahul Zaveri

measurements: Jerry Allwine, Chris Doran, Will Shaw, G-1 flight crew, ANL, BNL, and other NE-OPS participants

1999 NE-OPS Field Campaign



- wind profilers, **B**, **C** (ANL), **W** (PNNL), **R**, **F**
- sodar: **C** (ANL)
- radiosondes: **B** (ANL), **C** (PNNL)
- ozonesondes: **B** (PNNL)
- surface chemistry: **B**, **C** (ANL)
- tethersonde: **B**
- Raman lidar: **B**
- G-1 aircraft: (BNL)

DOE Atmospheric Chemistry Program

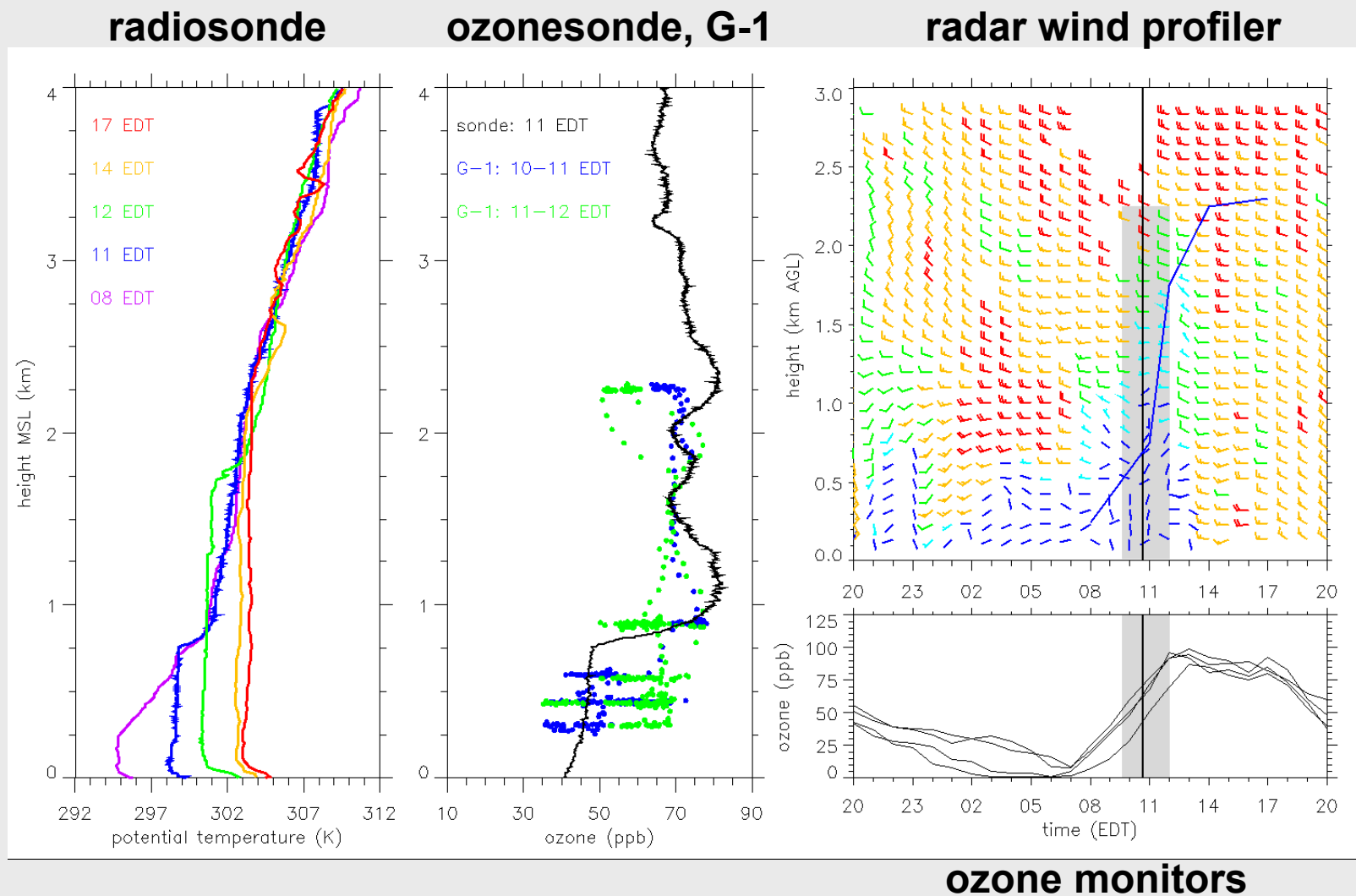
ANL - Argonne National Lab.

PNNL - Pacific Northwest National Lab.

BNL - Brookhaven National Lab.

http://www.pnl.gov/atmos.sciences/philadelphia_ex.html

Motivation: 5 August Observations



Model Description: PEGASUS

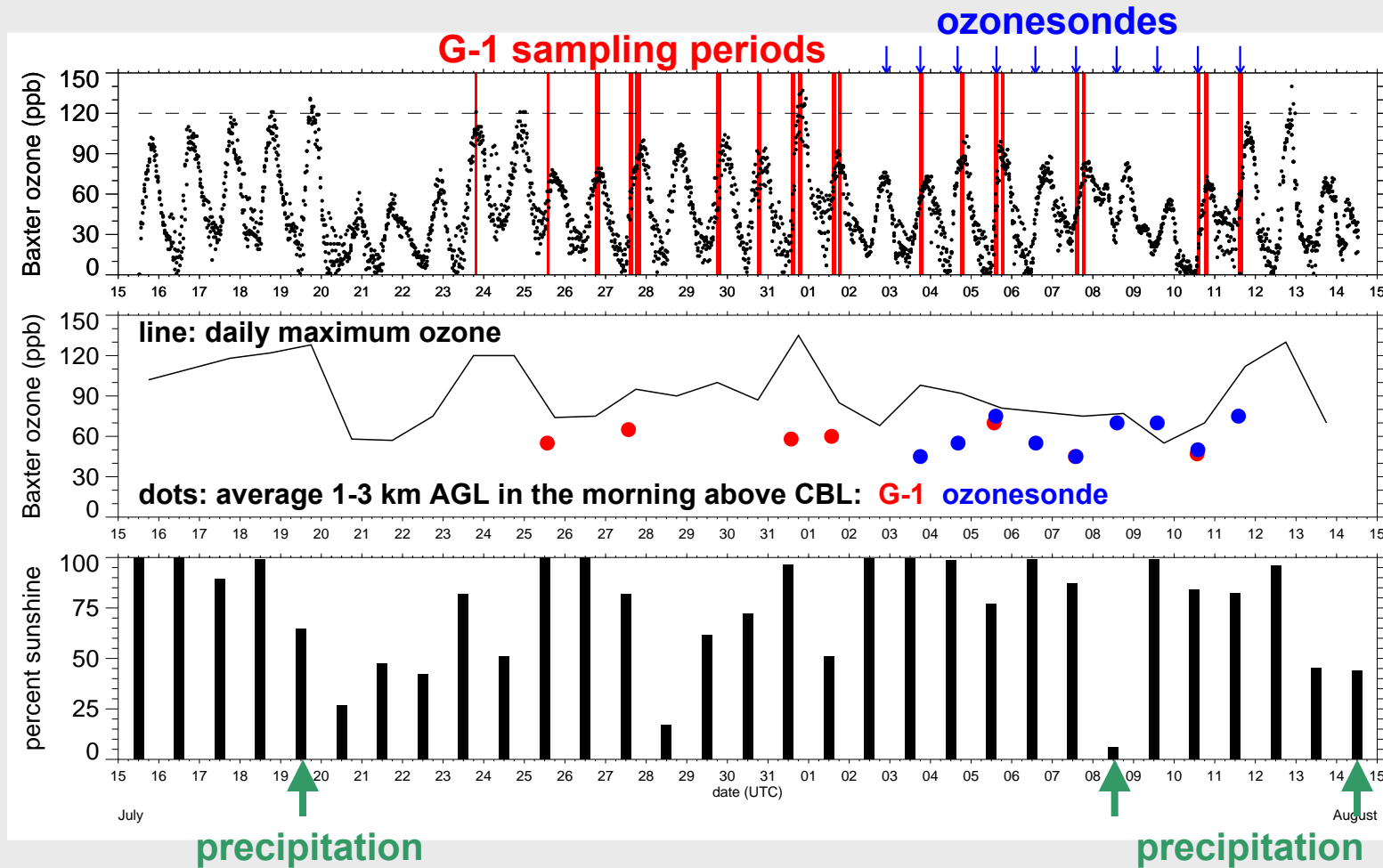
mesoscale meteorological model (RAMS)

- nested configuration: 48, 24, 8, and 4 km grids, $\Delta z_{\text{sfc}} = 25 \text{ m}$
- 30-day simulation period: 12 UTC 15 July - 12 UTC 14 August
- 4DDA on large-scale analyses
- clouds: form in areas of supersaturation

chemical transport model

- meteorological fields from RAMS, one-way coupling
- transport, vertical diffusion, chemical production/destruction, dry deposition, emission terms
- CBM-Z mechanism: 53 species and 133 reactions
- RODAS integrator
- photolysis rates modified by cloudiness
- day-specific emission rates on 8 levels from SMOKE (Jeff Vukovich, MCNC)

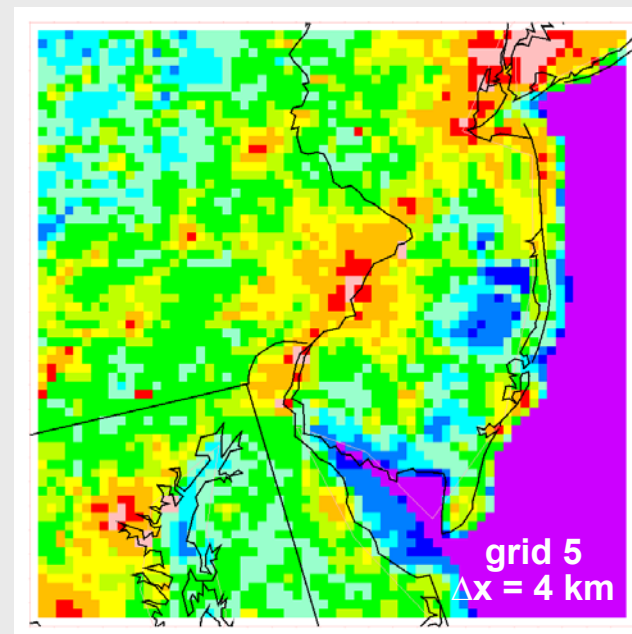
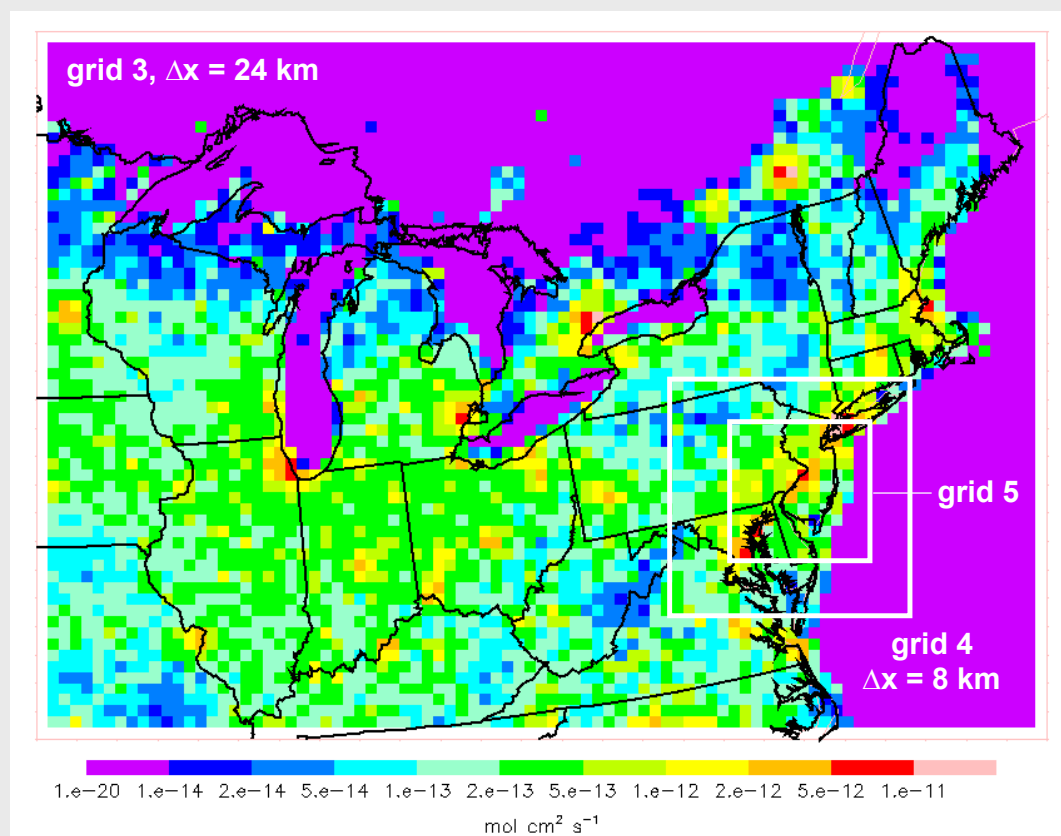
Data during Simulation Period



➡ trend in maximum surface ozone not correlated with limited data aloft

Model Domains

Surface NO_x Emission Rates, 12 UTC 15 July



(emissions aggregated from 4-km dataset)

Modeling Strategy

“Control” Simulation

Evaluate simulated meteorological and trace gas fields using
surface and upper-air observations

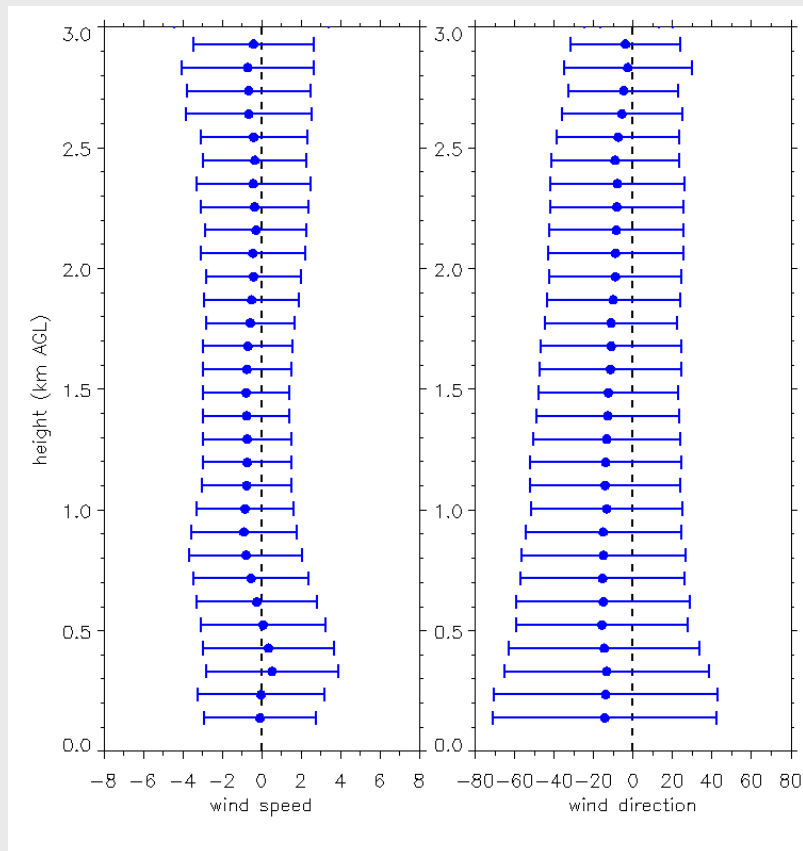
Qualitative assessment of regional-scale transport

“Sensitivity” Simulations

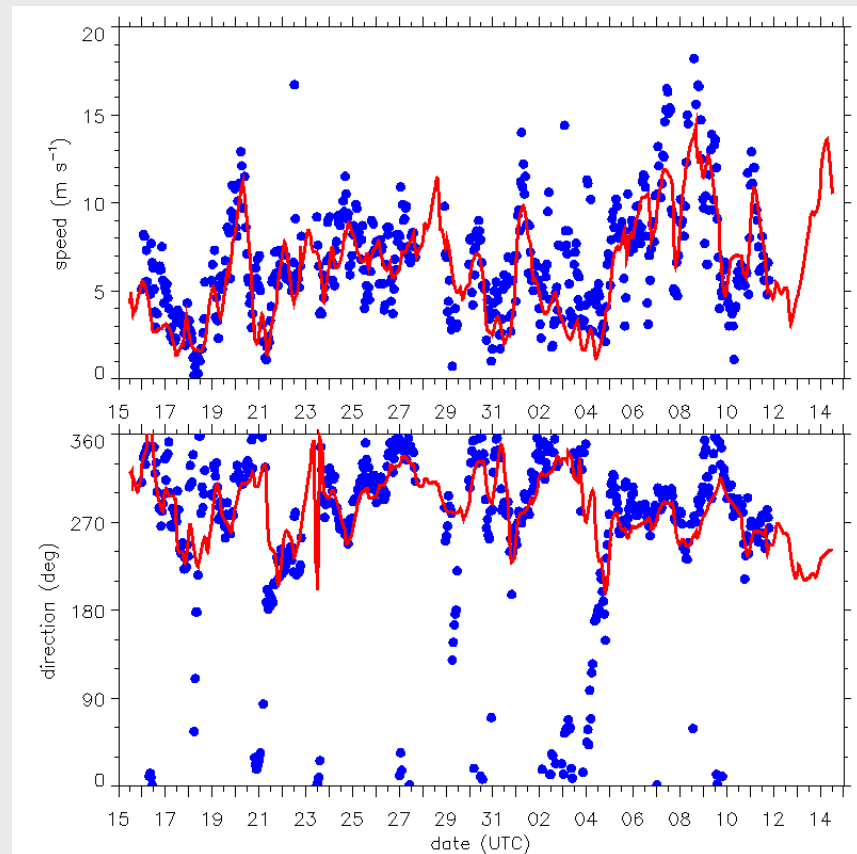
Quantitatively determine relative role of local and regional
processes

Evaluation: Upper-Air Winds

mean and standard deviation
of the bias (simulated - observed)

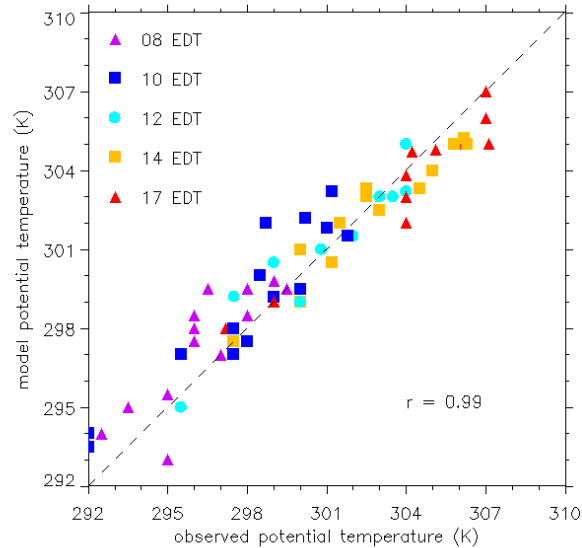


observed and simulated
~ 1.5 km AGL

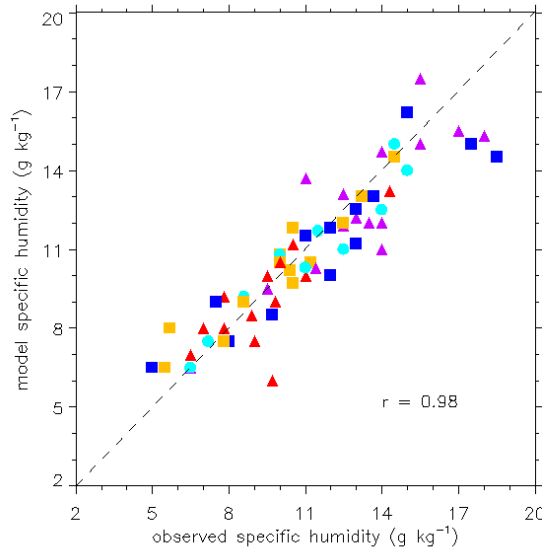


Evaluation: B-L Properties

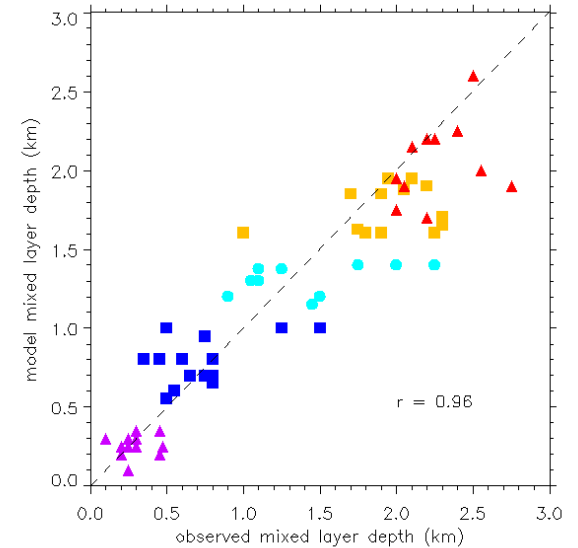
potential temperature



specific humidity



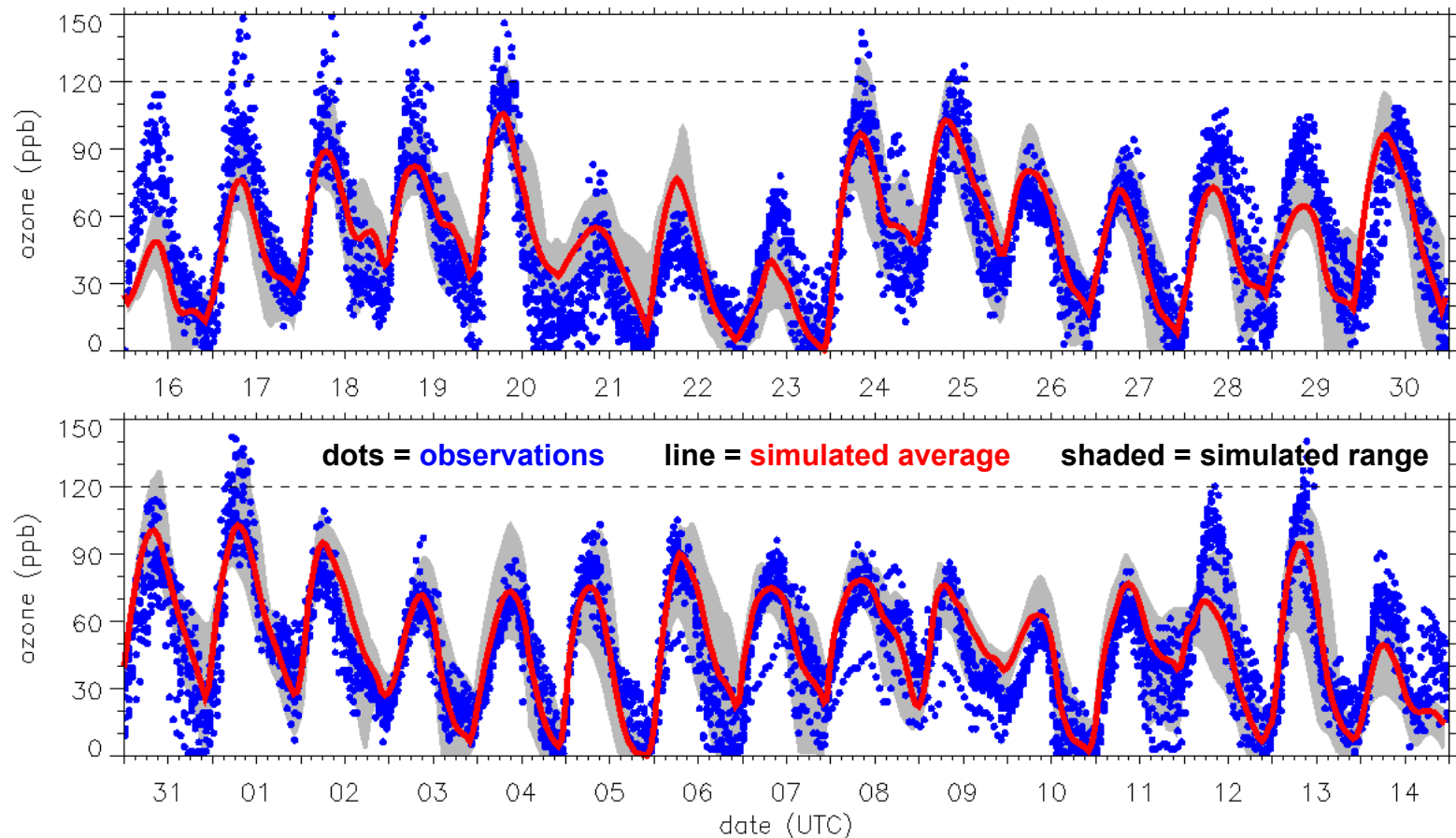
mixed layer depth



**observed values based on 65 radiosondes from site B
between 23 July and 11 August**

Evaluation: Surface Ozone

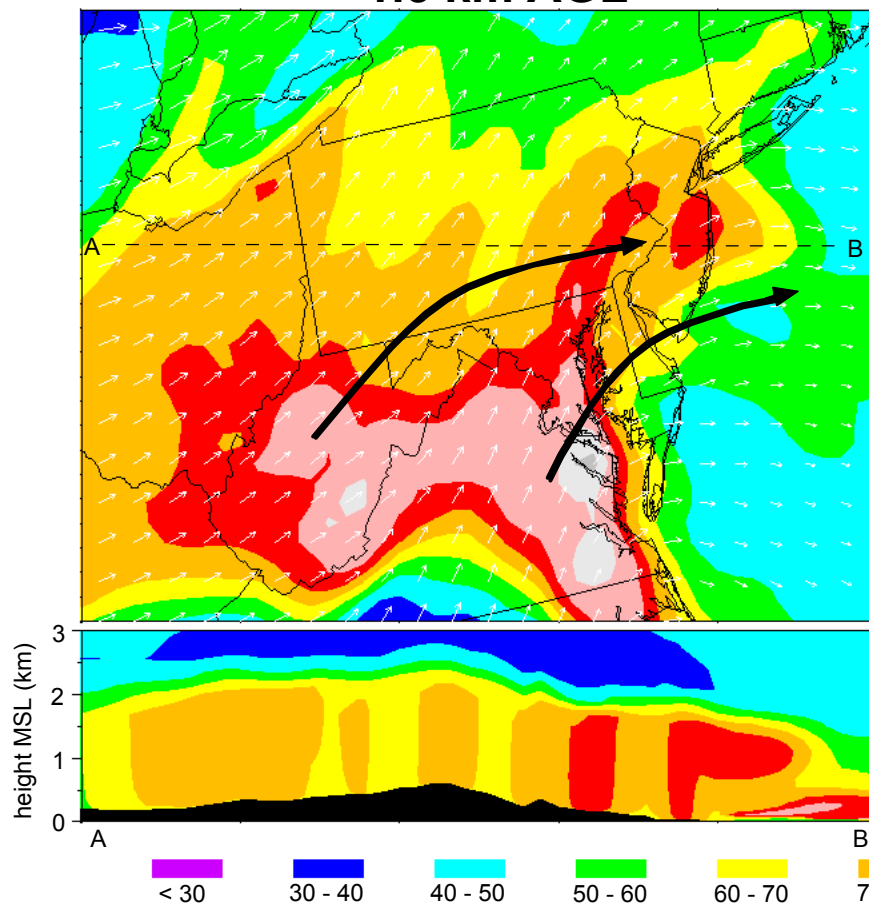
Observed and Simulated Ozone within 48 km of Philadelphia



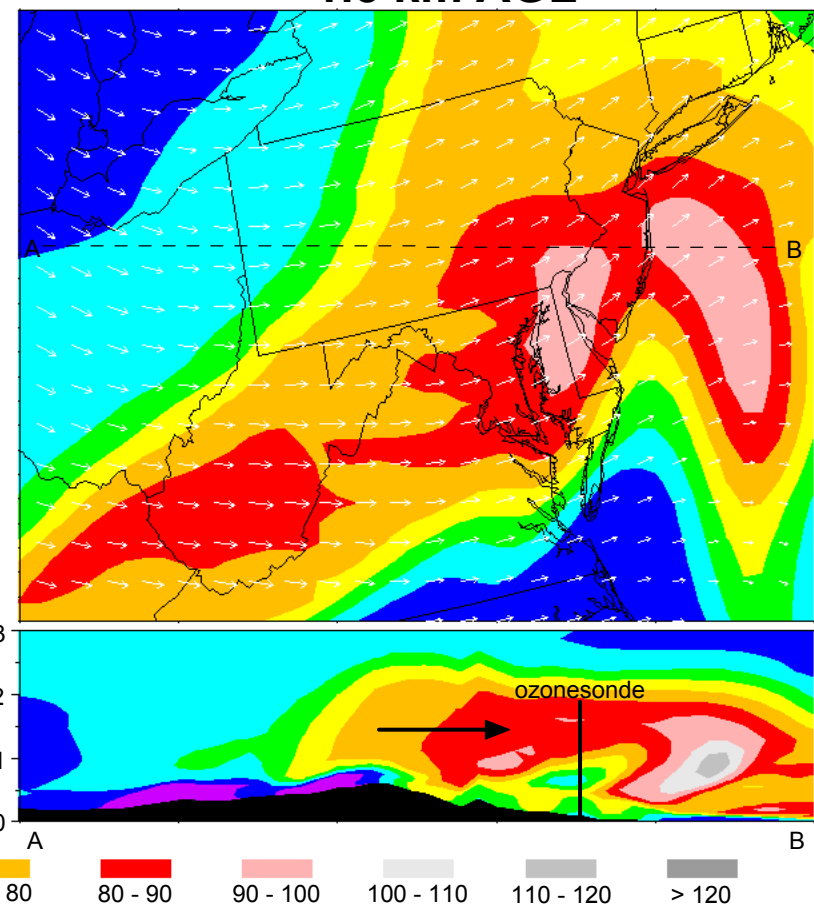
1-h max bias = -5.8	8-h max bias = -1.2	1-h min bias = 2.0
1-h max GE = 12.3	8-h max GE = 11.1	1-h min GE = 7.2

Regional Transport

17 EDT 10 August 1999
~ 1.5 km AGL

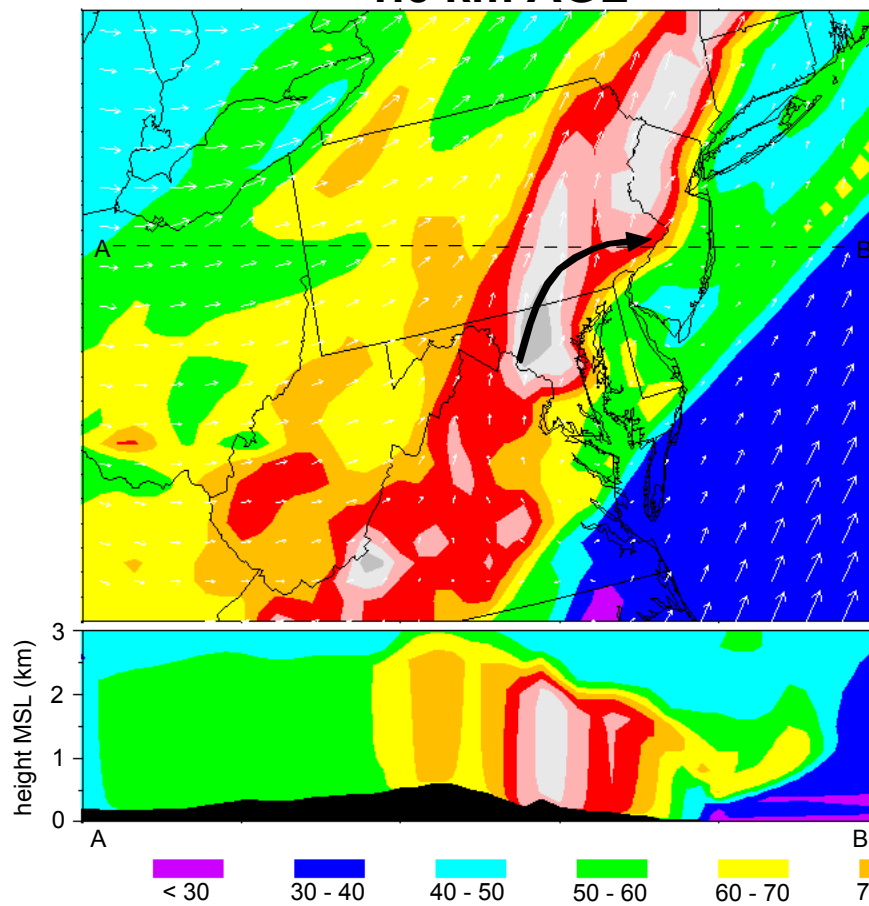


08 EDT 11 August 1999
~ 1.5 km AGL

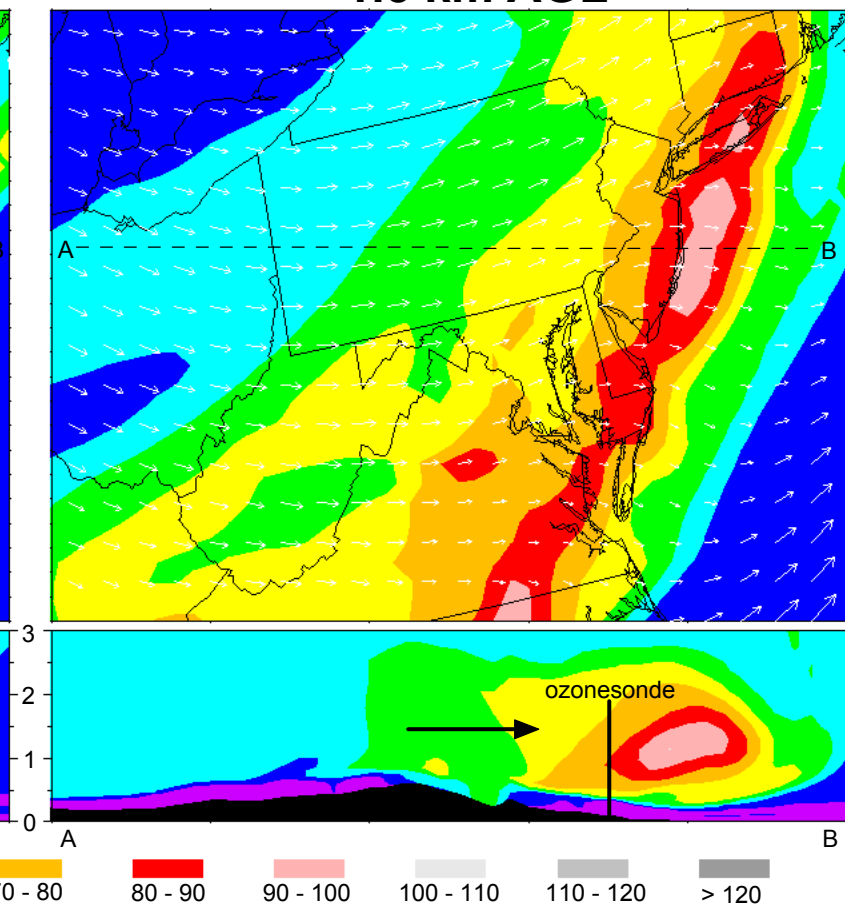


Regional Transport

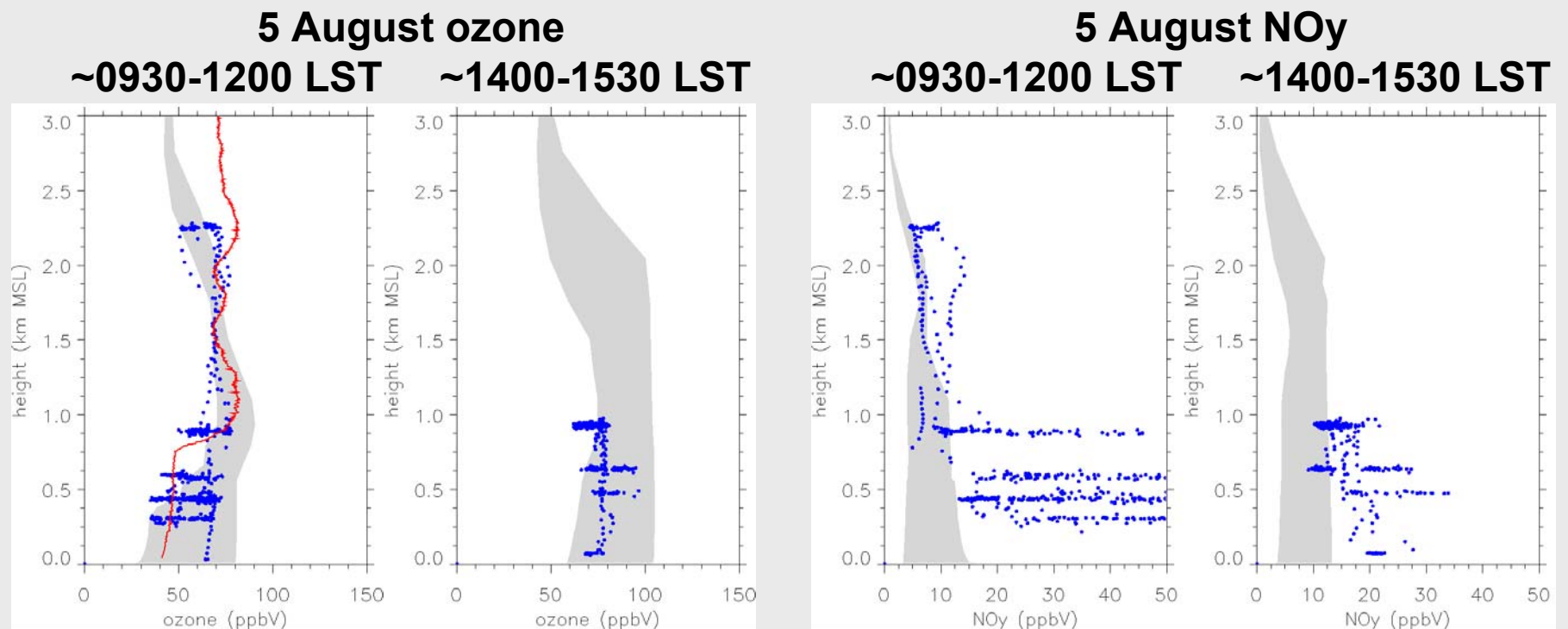
17 EDT 4 August 1999
~ 1.5 km AGL



08 EDT 5 August 1999
~ 1.5 km AGL



Ozone and NOy Aloft

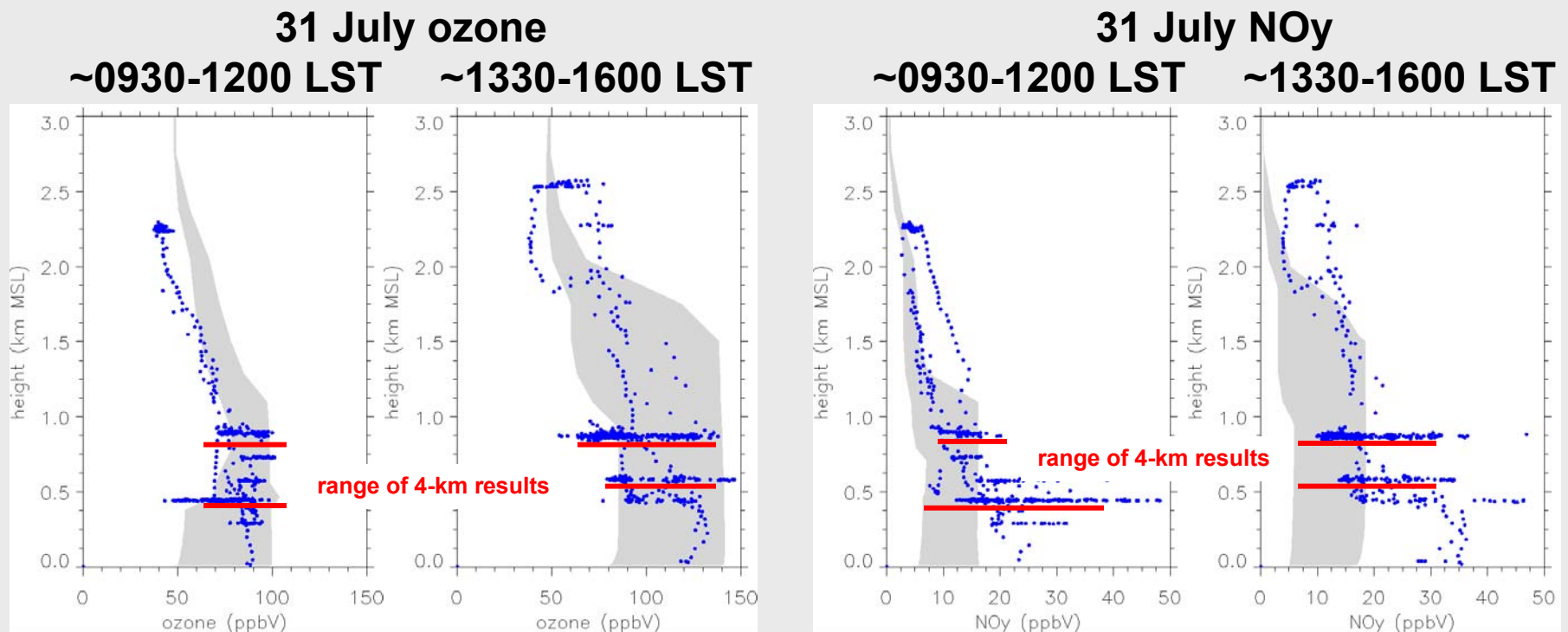


G-1

ozonesonde

shaded: range of 24-km model results within a vertical column encompassing the G-1 flight path and during the flight period

Ozone and NO_y Aloft

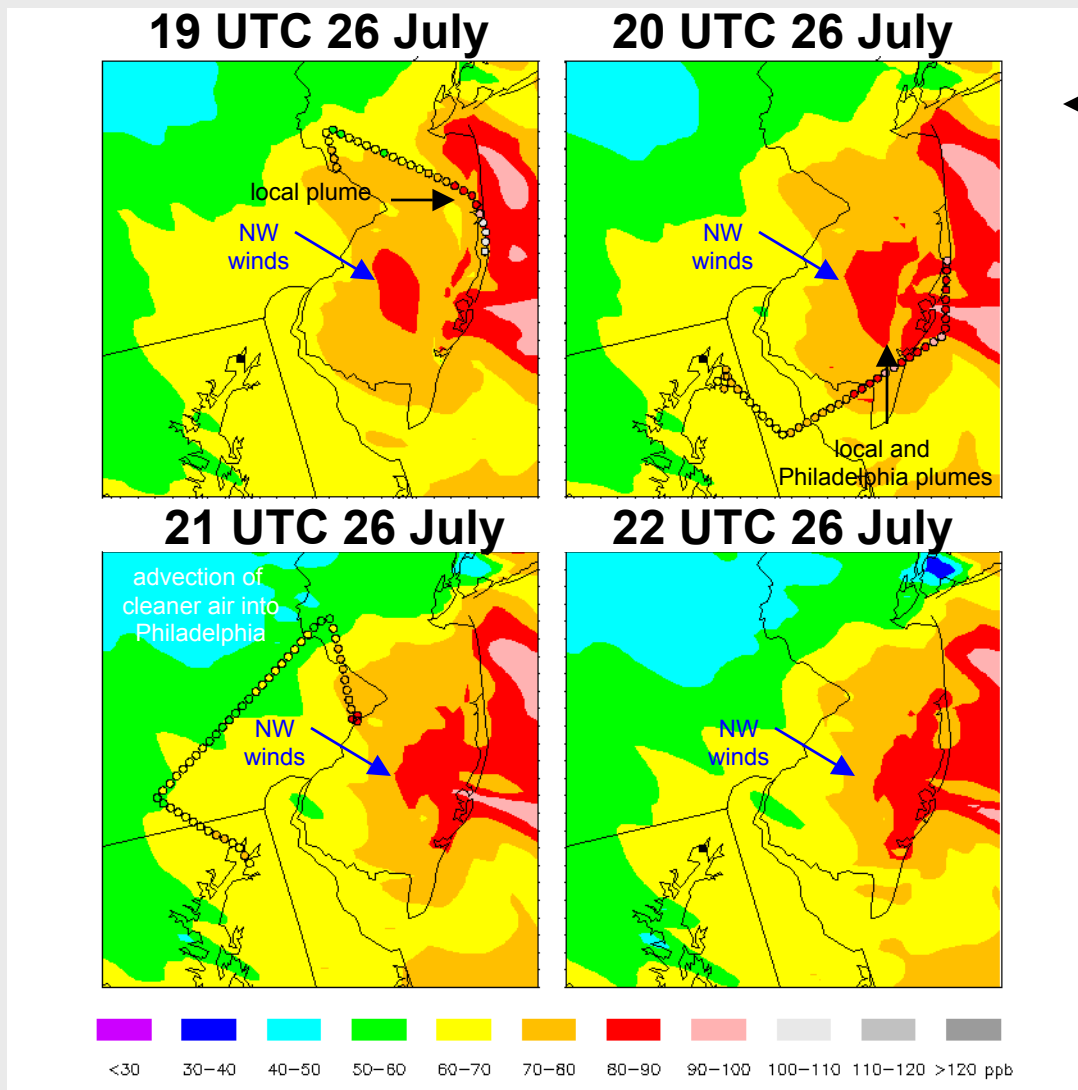


➔ 24 km and 4 km ozone similar, but NO_y better represented by 4 km

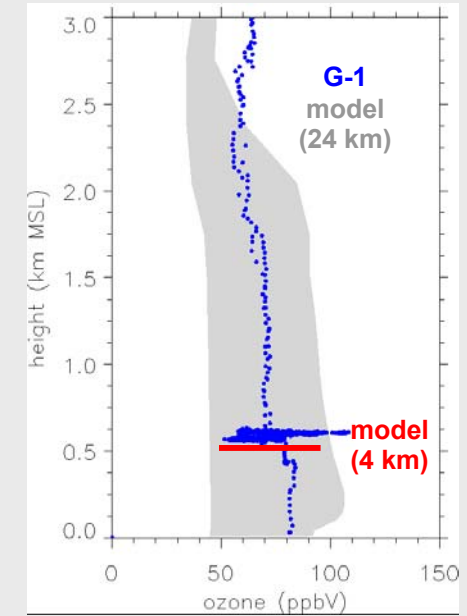
G-1

shaded: range of 24-km model results within a vertical column encompassing the G-1 flight path and during the flight period

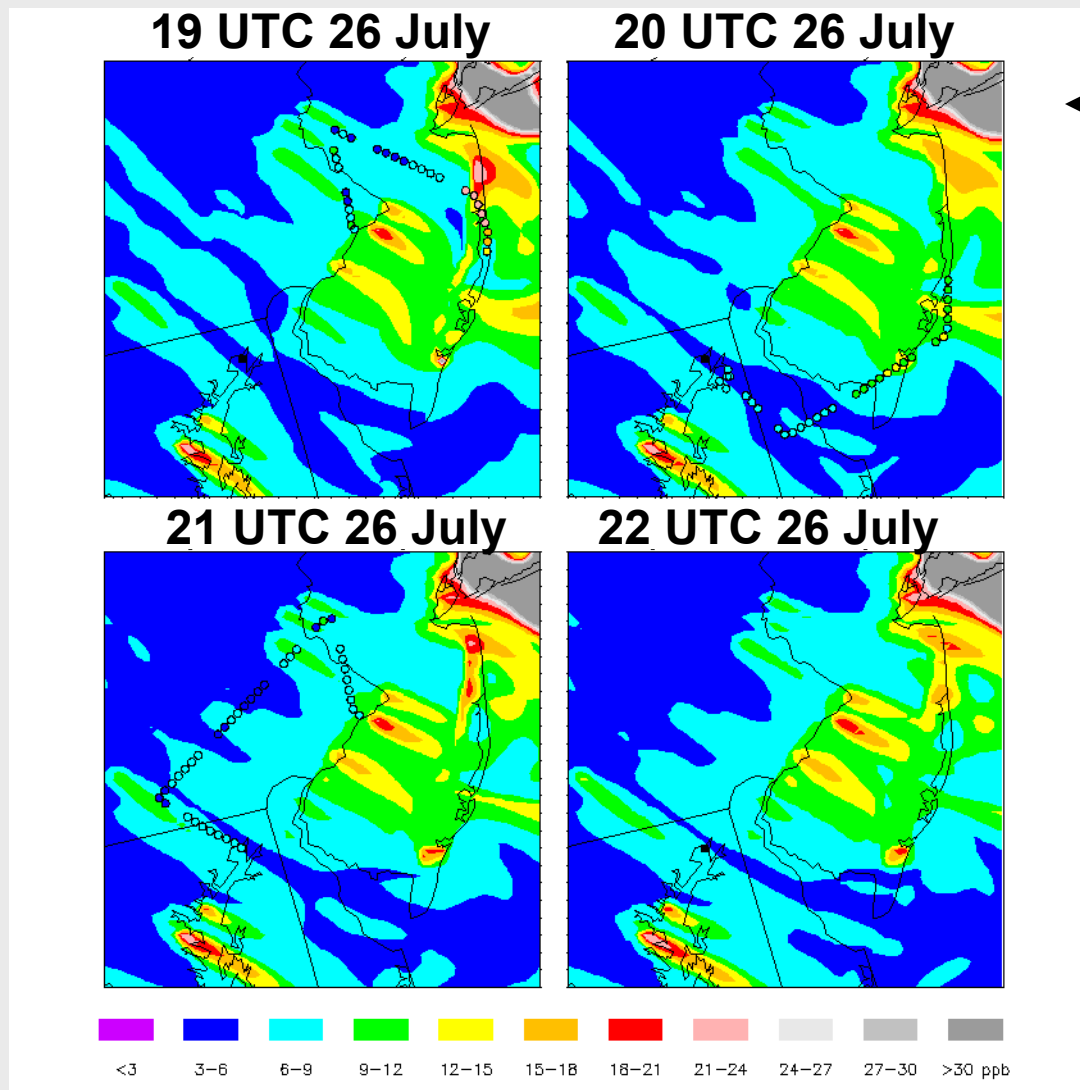
Local Transport: Ozone



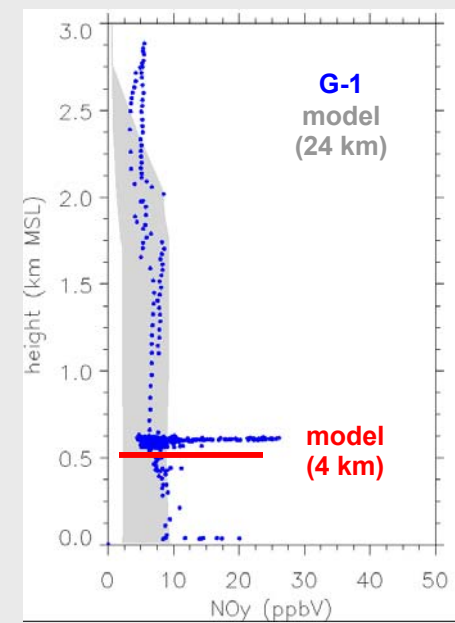
4-km simulation
~ 500 m AGL



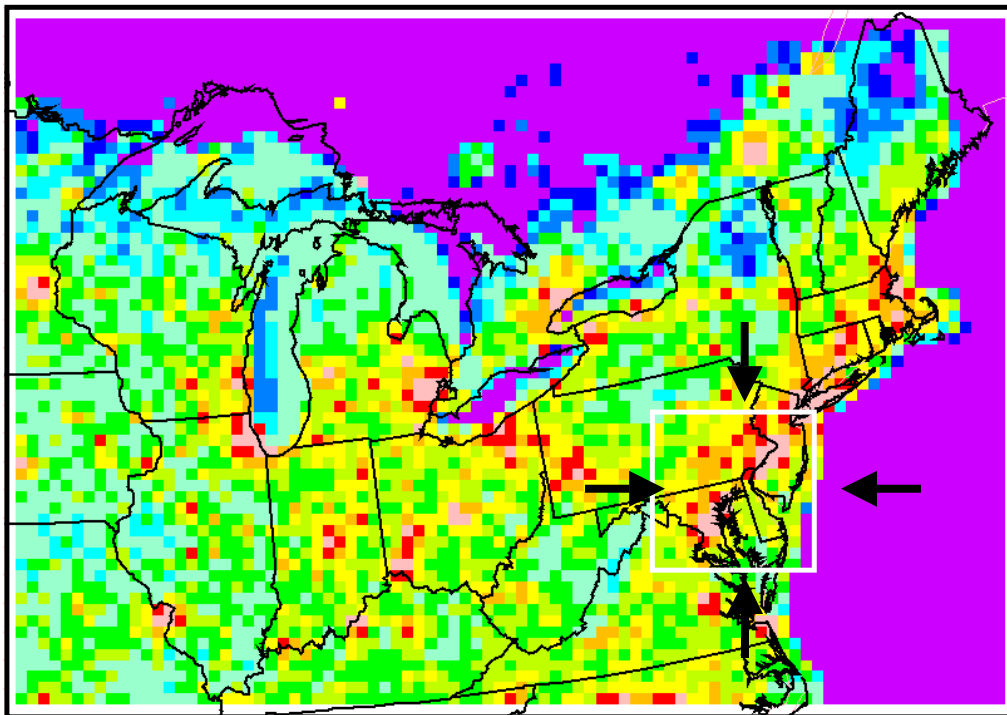
Local Transport: NO_y



4-km simulation
~ 500 m AGL



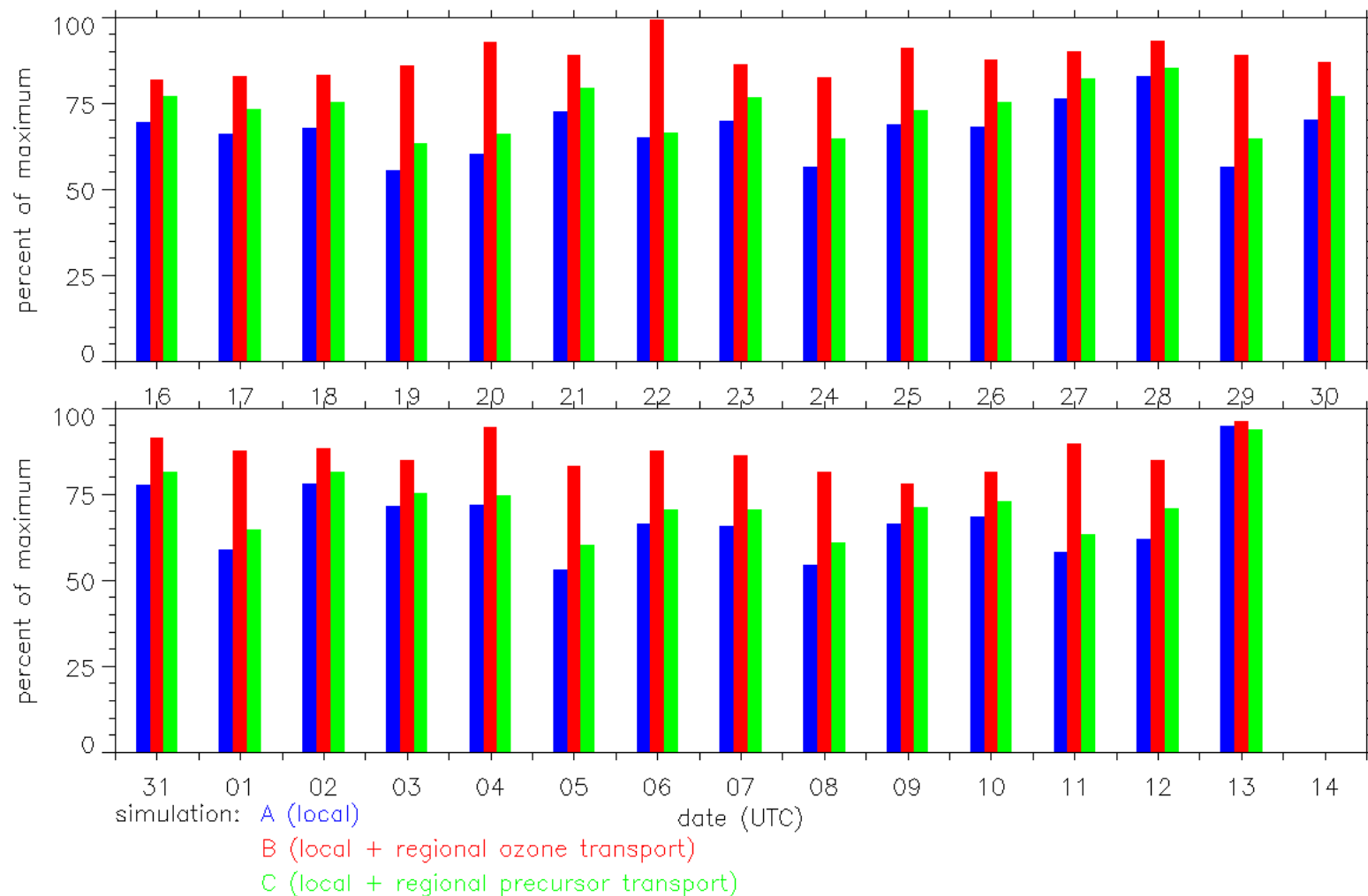
Sensitivity Simulations



$1. \times 10^{-20}$ $2. \times 10^{-14}$ $5. \times 10^{-14}$ $1. \times 10^{-13}$ $2. \times 10^{-13}$ $5. \times 10^{-13}$ $1. \times 10^{-12}$ $2. \times 10^{-12}$ $5. \times 10^{-12}$ $1. \times 10^{-11}$ $2. \times 10^{-11}$
 $\text{mol cm}^2 \text{s}^{-1}$

- 1) **local**
only emissions within subdomain, background values imported into subdomain
 - 2) **O_3 transport**
same as 1), but include regional O_3
 - 3) **O_3 precursor transport**
same as 1), but include regional O_3 precursors
- ➡ compare results with control simulation

Daily Peak Ozone Mixing Ratios



Summary

- data showed concentrations of ozone significantly higher above the growing CBL on several mornings
- PEGASUS results compared very well with meteorological and chemical data at the surface and aloft
 - ➔ O₃ from the 24 km and 4 km simulations similar, but O₃ precursors better represented by 4 km simulation
 - ➔ near-surface vertical grid spacing critical to adequately simulate the nocturnal boundary layer
- sensitivity simulations showed that the majority of ozone was produced by emissions in Philadelphia and Chesapeake Bay area, but as much as 30-40% of the ozone could be attributed to transport from upwind sources
 - ➔ simulated regional pollutant plumes were not completely aged
 - ➔ several source regions usually contributed to the mix of pollutants